



chain nodes :

16 17 18 25 26 27 28

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 19 20 21 22 23 24

chain bonds :

6-7 13-16 14-26 16-17 17-18 17-25 18-19 18-28 23-27

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-9 8-11 9-10 10-12 11-12 11-13 12-15 13-14 14-15
19-21 19-22 20-21 20-23 22-24 23-24

exact/norm bonds :

11-13 12-15 13-14 13-16 14-15 14-26 17-18 17-25 18-19

exact bonds :

6-7 16-17 18-28 23-27

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-9 8-11 9-10 10-12 11-12 19-21 19-22 20-21 20-23
22-24 23-24

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 28:CLASS